

Supplementary Information

Electrospray Ionization Mass Spectrometry Fingerprinting of Extracts of the Leaves of *Arrabidaea chica*

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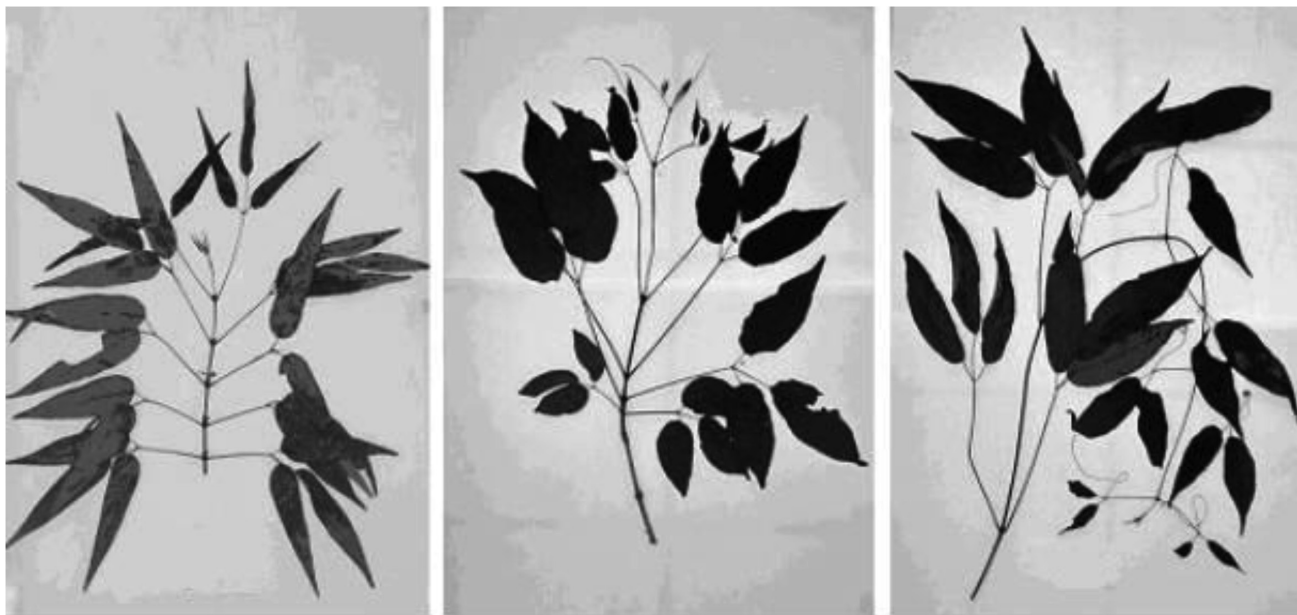


Figure S1. Dried *A. chica* leaves of varieties (a) I, (b) II and (c) III.

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Figure S2. Fresh *A. chica* leaves of varieties (a) I, (b) II and (c) III.

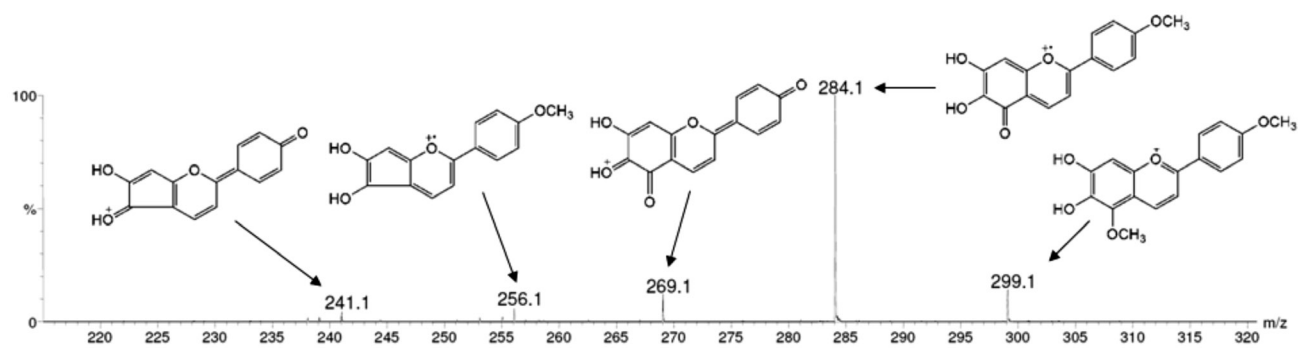
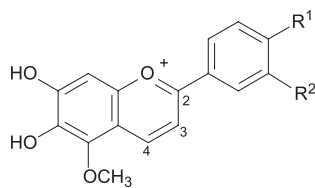


Figure S3. ESI(+)-MS/MS of the cationic 3-deoxyanthocyanidin **2** (m/z 299). Suggestions for the structure of major fragment ions are shown.

Table S1. Cationic 3-deoxyanthocyanidins **1-4** found in *A. chica*



3-deoxyanthocyanidin	R ₁	R ₂	m/z [M ⁺]
1	OH	H	285
2	OCH ₃	H	299
3	OH	OH	301
4	OCH ₃	OH	315

Table S2. continuation

	Variety I - Mass to charge ratios and data on relative signal intensities from the mass spectral analyses of the three varieties of <i>A. chica</i> (20% least intense were excluded)															
	ACI_C_Ma	ACI_C_La	ACI_C_Aa	ACI_S_Ma	ACI_S_La	ACI_S_Aa	ACI_C_Mb	ACI_C_Lb	ACI_C_Ab	ACI_S_Mb	ACI_S_Lb	ACI_S_Ab	Range (min/max)	AVG	SD	
351.1																
357.2	8.0	7.2	7.6	2.6	8.0	2.1	9.3	7.2	6.7	1.9	5.9	1.6	1.6	9.3	5.7	2.8
357.3																
365.1																
365.2																
369.4																
371.2																
373.2																
381.1	0.0	0.0	0.0	0.0	0.0	1.3	1.5	0.0	1.2	0.0	1.5	1.5	0.0	1.5	0.6	0.7
393.2																
409.2																
427.1	1.8	0.0	0.0	0.0	1.4	1.2	1.5	0.0	0.0	0.0	0.0	0.0	0.0	1.8	0.5	0.7
427.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.0	0.9	0.1	0.3
431.4																
437.2																
437.3																
442.3	0.0	0.0	1.2	0.0	2.6	0.0	0.0	0.0	1.2	0.0	2.2	0.0	0.0	2.6	0.6	1.0
447.1	1.9	1.8	1.5	0.0	0.0	0.0	1.1	1.3	0.0	0.0	0.0	0.0	0.0	1.9	0.6	0.8
455.4	0.0	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.1	0.3
459.5																
461.2																
463.1	16.6	14.4	15.6	3.1	18.8	2.5	14.8	11.8	13.1	2.8	13.0	2.0	2.0	18.8	10.7	6.3
473.4	0.0	0.0	0.0	0.9	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9	0.1	0.3
477.1																
477.2	10.9	7.8	8.6	1.6	10.4	1.5	9.4	7.1	7.3	1.1	6.6	1.0	1.0	10.9	6.1	3.8
479.2																
485.1																
485.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	1.0	0.1	0.3
485.9																
493.2																
495.9																
501.1	1.0	1.0	1.0	0.0	1.2	0.0	0.9	0.9	0.8	0.0	0.8	0.0	0.0	1.2	0.6	0.5
517.1																
517.2	1.2	1.2	1.1	0.0	1.4	0.0	1.1	1.0	1.2	0.0	1.4	0.0	0.0	1.4	0.8	0.6
519.1	0.0	2.0	2.2	0.0	2.4	0.0	0.0	0.0	0.0	0.0	1.8	0.0	0.0	2.4	0.7	1.0
519.2	0.0	0.0	0.0	0.0	0.0	0.0	2.5	2.1	1.7	0.0	0.0	0.0	0.0	2.5	0.5	1.0

Table S2. continuation

	Variety III - Mass to charge ratios and data on relative signal intensities from the mass spectral analyses of the three varieties of <i>A. chitica</i> (20% least intense were excluded)																AVG	SD
	AC3_C_Ma	AC3_C_La	AC3_C_Aa	AC3_S_Ma	AC3_S_La	AC3_S_Aa	AC3_C_Mb	AC3_C_Lb	AC3_C_Ab	AC3_S_Mb	AC3_S_Lb	AC3_S_Ab	Range(min/max)					
158.1																		
160.1	10.3	14.2	12.5	12.1	14.4	15.0	12.0	16.1	13.4	13.4	12.7	13.4	18.7	10.3	18.7	13.7	2.2	
161.0																		
164.1	9.4	11.1	10.4	8.1	10.7	13.2	11.1	13.0	11.5	11.5	9.3	10.2	16.6	8.1	16.6	11.2	2.2	
193.0																		
203.1	6.7	4.7	0.0	4.5	0.0	0.0	4.8	4.3	0.0	0.0	4.1	4.6	0.0	0.0	6.7	2.8	2.6	
207.0																		
217.1																		
229.1																		
231.1	0.0	0.0	0.0	0.0	0.0	3.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.2	0.3	0.9	
233.1																		
239.2																		
243.1	4.9	0.0	0.0	3.0	0.0	0.0	0.0	0.0	0.0	0.0	2.3	0.0	0.0	0.0	4.9	0.9	1.6	
261.1	3.1	0.0	0.0	2.3	0.0	0.0	2.7	0.0	0.0	0.0	0.0	3.1	0.0	0.0	3.1	0.9	1.4	
261.2																		
271.1	4.1	0.0	0.0	3.3	0.0	0.0	0.0	0.0	0.0	0.0	2.8	0.0	0.0	0.0	4.1	0.8	1.6	
277.1																		
279.3	0.0	0.0	0.0	1.9	0.0	0.0	0.0	0.0	0.0	0.0	1.8	0.0	0.0	0.0	1.9	0.3	0.7	
280.1																		
283.2																		
285.1	5.8	6.0	0.0	7.3	6.7	6.0	8.6	5.9	4.0	4.0	7.2	6.2	6.0	0.0	8.6	5.8	2.1	
287.1	0.0	0.0	5.2	9.6	0.0	0.0	20.5	9.0	5.5	5.5	10.6	5.8	5.3	0.0	20.5	6.0	6.0	
299.1	8.5	11.0	0.0	8.0	5.2	5.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	11.0	3.2	4.2	
301.1	14.8	14.8	8.9	21.2	19.3	18.1	0.0	16.0	10.4	10.4	21.7	16.6	17.8	0.0	21.7	15.0	6.1	
303.1	0.0	0.0	11.1	0.0	0.0	1.9	8.3	0.0	10.8	10.8	0.0	2.2	0.0	0.0	11.1	2.9	4.5	
305.2																		
315.1	4.3	4.8	0.0	7.5	5.4	6.0	4.3	5.0	3.4	3.4	7.7	4.9	6.4	0.0	7.7	5.0	2.0	
317.1	0.0	0.0	3.6	0.0	0.0	0.0	0.0	0.0	3.6	3.6	0.0	0.0	0.0	0.0	3.6	0.6	1.4	
321.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3	0.0	0.0	0.0	1.3	0.1	0.4	
322.1																		
327.2																		
331.1	0.0	0.0	0.0	1.7	0.0	0.0	0.0	0.0	0.0	0.0	1.6	0.0	0.0	0.0	1.7	0.3	0.6	
333.1	2.0	0.0	0.0	1.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.0	0.3	0.7	
340.2																		
341.4	0.0	0.0	3.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.5	0.3	1.0	
349.2																		
351.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.2	0.0	1.2	0.1	0.3	

Table S2. continuation

	Variety III - Mass to charge ratios and data on relative signal intensities from the mass spectral analyses of the three varieties of <i>A. chitica</i> (20% least intense were excluded)														AVG	SD
	AC3_C_Ma	AC3_C_La	AC3_C_Aa	AC3_S_Ma	AC3_S_La	AC3_S_Aa	AC3_C_Mb	AC3_C_Lb	AC3_C_Ab	AC3_S_Mb	AC3_S_Lb	AC3_S_Ab	Range(min/max)			
533.2	1.0	0.9	1.4	0.0	1.3	1.0	0.9	0.8	1.2	0.0	1.2	0.9	0.0	1.4	0.9	0.4
547.1																
547.2																
549.2	1.0	0.8	1.6	0.0	1.6	1.0	0.8	0.7	0.9	0.0	1.4	1.1	0.0	1.6	0.9	0.5
563.2																
565.1																
565.2																
571.2																
577.2																
579.2	0.0	0.0	0.8	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8	0.1	0.3
583.2																
585.2	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.5	0.0	0.0	0.0	0.5	0.1	0.2
593.3	0.0	0.0	2.4	0.0	0.0	0.0	2.0	3.0	1.8	3.6	3.1	2.1	0.0	3.6	1.5	1.4
593.4	2.1	2.9	0.0	3.4	2.7	2.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.4	1.1	1.4
599.2	0.0	0.0	0.0	0.8	0.0	0.0	0.7	0.5	0.0	0.8	0.0	0.0	0.0	0.8	0.2	0.3
599.3																
603.2																
607.2																
609.3	0.0	1.1	0.9	1.2	0.8	0.9	0.0	0.0	0.0	1.2	0.0	0.9	0.0	1.2	0.6	0.5
617.2																
617.3																
637.2																
637.4	0.0	0.0	0.0	0.0	0.0	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.0	0.1
643.3																
645.3																
657.3																
709.22																
869.34																
Highest intensity ion	14.8	14.8	12.5	21.2	19.3	18.1	20.5	16.1	13.4	21.7	16.6	18.7	301.0	301.0	160.0	160.0
	301.0	301.0	160.0	301.0	301.0	301.0	287.0	160.0	160.0	301.0	301.0	160.0	301.0	301.0	160.0	160.0